ELSEVIER

Chemical Physics 218 (1997) 341–344

Chemical Physics

Author index to volume 218

Alikhani, M.E., see Tremblay, B. 218 (1997) 37
Alonso, J.L., F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler, Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex 218 (1997) 267
Antoine, R., see Dugourd, Ph. 218 (1997) 163
Au, J.W. and C.E. Brion, Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide 218 (1997) 109
Au, J.W. and C.E. Brion, Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions 218 (1997) 87

Bagnich, S.A., The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses 218 (1997) 277
Boilot, J.P., see Brunel, M. 218 (1997) 301
Borsenberger, P.M., see Sinicropi, J.A. 218 (1997) 331
Brion, C.E., see Au, J.W. 218 (1997) 109
Brion, C.E., see Au, J.W. 218 (1997) 87
Brion, C.E., see Olney, T.N. 218 (1997) 127
Broyer, M., see Dugourd, Ph. 218 (1997) 163
Brun, A., see Brunel, M. 218 (1997) 301
Brunel, M., F. Chaput, S.A. Vinogradov, B. Campagne, M. Canva, J.P. Boilot and A. Brun, Reverse saturable absorption in palladium and zinc tetraphenyltetrabenzoporphyrin doped xerogels 218 (1997) 301
Buijsse, B., see Wouters, E.R. 218 (1997) 309
Buonomo, E., F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal, A full quantum study of the vibrational predissociation mechanisms in Ar_3^+ cluster 218 (1997) 71
Burton, G.R., see Olney, T.N. 218 (1997) 127

Campagne, B., see Brunel, M. 218 (1997) 301
Canva, M., see Brunel, M. 218 (1997) 301
Chan, W.F., see Olney, T.N. 218 (1997) 127
Chaput, F., see Brunel, M. 218 (1997) 301
Chowdhury, P.K., see Schmid, R.P. 218 (1997) 291
Christen, C., see Dietz, F. 218 (1997) 43
Chua, M. and P.A. Tanner, Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $Cs_2NaCeCl_6$ 218 (1997) 83
Cooper, G., see Olney, T.N. 218 (1997) 127

Cowdery-Corvan, J.R., see Sinicropi, J.A. 218 (1997) 331
Cuadros, F., A. Mulero and W. Okrasinski, Thermodynamic shift from three- to two-dimensional systems 218 (1997) 235

Delgado-Barrio, G., see Buonomo, E. 218 (1997) 71
DeWitt, M.J., D.W. Peters and R.J. Levis, Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation 218 (1997) 211
Dietz, F., N. Tyutyulkov, C. Christen and K. Lüders, Nature of the magnetic interaction of Wurster's radicals in the solid state 218 (1997) 43
Ding, S., see Guan, D. 218 (1997) 1
Dreizler, H., see Alonso, J.L. 218 (1997) 267
Dugourd, Ph., D. Rayane, R. Antoine and M. Broyer, Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process 218 (1997) 163
Dyke, J.M., see Mack, P. 218 (1997) 243

Evangelisti, S., Carbon–oxygen clusters as hypothetical high energy-density materials 218 (1997) 21

Fišer, J., see Vojtík, J. 218 (1997) 13

Gianturco, F.A., see Buonomo, E. 218 (1997) 71
Guan, D., X. Yi, S. Ding and B. Yang, Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface 218 (1997) 1

Hawlicka, E. and D. Swiatla-Wojcik, Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components 218 (1997) 49
Hirao, K., see Tajima, N. 218 (1997) 257
Hiraya, A., see Kanda, K. 218 (1997) 199
Hu, Y., W. Lu and S. Yang, Intermolecular vibrations of the van der Waals complex p-$C_6H_4FCH_3 \ldots Ar$ 218 (1997) 325

Ito, F., see Schmid, R.P. 218 (1997) 291

Jones, H., see Schmid, R.P. 218 (1997) 291

Kanda, K., S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake, Photodissociation spectroscopy of ICN in the vacuum ultraviolet region 218 (1997) 199
Katsumata, S., see Kanda, K. 218 (1997) 199
Kondow, T., see Kanda, K. 218 (1997) 199
Küster, J., see Schael, F. 218 (1997) 175

Lesarri, A., see Alonso, J.L. 218 (1997) 267
Levis, R.J., see DeWitt, M.J. 218 (1997) 211
Löhmannsröben, H.-G., see Schael, F. 218 (1997) 175
López, J.C., see Alonso, J.L. 218 (1997) 267
Lorenzo, F.J., see Alonso, J.L. 218 (1997) 267
Lu, W., see Hu, Y. 218 (1997) 325
Lüders, K., see Dietz, F. 218 (1997) 43

Mack, P., J.M. Dyke and T.G. Wright, Calculated thermodynamics of reactions involving $NO^+ \cdot X$ complexes (where $X = H_2O$, N_2 and CO_2) 218 (1997) 243
Magin, E.H., see Sinicropi, J.A. 218 (1997) 331
Manceron, L., see Tremblay, B. 218 (1997) 37
Mata, S., see Alonso, J.L. 218 (1997) 267
Mataras, D., see Stamou, S. 218 (1997) 57
Maus, M. and W. Rettig, The electronic structure of 4-(N,N-dimethylamino)-4′-cyano-biphenyl and its planar and twisted model compounds 218 (1997) 151
Mets, Ü., J. Widengren and R. Rigler, Application of the antibunching in dye fluorescence: measuring the excitation rates in solution 218 (1997) 191
Miret-Artés, S., see Buonomo, E. 218 (1997) 71
Miyawaki, J., see Schmid, R.P. 218 (1997) 291
Mulero, A., see Cuadros, F. 218 (1997) 235

Nagata, T., see Kanda, K. 218 (1997) 199
Nakanaga, T., see Schmid, R.P. 218 (1997) 291

Okrasinski, W., see Cuadros, F. 218 (1997) 235
Olney, T.N., G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan, Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique 218 (1997) 127

Peters, D.W., see DeWitt, M.J. 218 (1997) 211
Pilar de Lara, M., see Buonomo, E. 218 (1997) 71

Rapakoulias, D., see Stamou, S. 218 (1997) 57
Rayane, D., see Dugourd, Ph. 218 (1997) 163
Reid, K.L., see Wouters, E.R. 218 (1997) 309
Rettig, W., see Maus, M. 218 (1997) 151
Rigler, R., see Mets, Ü. 218 (1997) 191

Schael, F., J. Küster and H.-G. Löhmannsröben, The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates 218 (1997) 175
Schmid, R.P., P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones, Infrared spectroscopy of aniline–X ($X = N_2$, CH_4, CHF_3, CO) clusters and their corresponding cluster cations in the NH_2-stretching vibration region 218 (1997) 291
Shobatake, K., see Kanda, K. 218 (1997) 199
Siebbeles, L.D.A., see Wouters, E.R. 218 (1997) 309
Sinicropi, J.A., J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger, Hole transport in vapor deposited enamines and enamine doped polymers 218 (1997) 331
Small, G.J., see Wu, H.-M. 218 (1997) 225
Stamou, S., D. Mataras and D. Rapakoulias, Simulation of the SiH ($A^2\Delta \rightarrow X^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants 218 (1997) 57
Stefanovich, E.V., see Truong, T.N. 218 (1997) 31
Sugawara, K., see Schmid, R.P. 218 (1997) 291
Swiatla-Wojcik, D., see Hawlicka, E. 218 (1997) 49

Tabayashi, K., see Kanda, K. 218 (1997) 199
Tajima, N., T. Taketsugu and K. Hirao, Theoretical study on adsorption and proton exchange reaction of H_2O on H-form zeolite 218 (1997) 257
Takeo, H., see Schmid, R.P. 218 (1997) 291
Taketsugu, T., see Tajima, N. 218 (1997) 257
Tan, K.H., see Olney, T.N. 218 (1997) 127
Tanner, P.A., see Chua, M. 218 (1997) 83
Tremblay, B., M.E. Alikhani and L. Manceron, Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study 218 (1997) 37
Truong, T.N. and E.V. Stefanovich, Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential 218 (1997) 31
Tyutyulkov, N., see Dietz, F. 218 (1997) 43

Van der Zande, W.J., see Wouters, E.R. 218 (1997) 309
Villarreal, P., see Buonomo, E. 218 (1997) 71
Vinogradov, S.A., see Brunel, M. 218 (1997) 301
Vojtík, J. and J. Fišer, Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH^- and NeH^+ 218 (1997) 13

Widengren, J., see Mets, Ü. 218 (1997) 191
Wouters, E.R., L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande, Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H_2 218 (1997) 309
Wright, T.G., see Mack, P. 218 (1997) 243
Wu, H.-M. and G.J. Small, Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores 218 (1997) 225

Yang, B., see Guan, D. 218 (1997) 1
Yang, S., see Hu, Y. 218 (1997) 325
Yi, X., see Guan, D. 218 (1997) 1

ELSEVIER

Chemical Physics 218 (1997) 345–353

Chemical Physics

Subject index to volume 218

Methods

Theoretical

Group theory and algebras

Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1

Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225

Many body and quasiparticle approaches

Thermodynamic shift from three- to two-dimensional systems, F. Cuadros, A. Mulero and W. Okrasinski 218 (1997) 235

Ab initio schemes for stationary properties

Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH^- and NeH^+, J. Vojtík and J. Fišer 218 (1997) 13

Carbon–oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21

Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31

Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study, B. Tremblay, M.E. Alikhani and L. Manceron 218 (1997) 37

Calculated thermodynamics of reactions involving $NO^+ \cdot X$ complexes (where $X = H_2O$, N_2 and CO_2), P. Mack, J.M. Dyke and T.G. Wright 218 (1997) 243

Computational and simulation methods

Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31

Nature of the magnetic interaction of Wurster's radicals in the solid state, F. Dietz, N. Tyutyulkov, C. Christen and K. Lüders 218 (1997) 43

Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49

Simulation of the SiH ($A^2\Delta \rightarrow X\,^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulias 218 (1997) 57

Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225
Theoretical study on adsorption and proton exchange reaction of H_2O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257

Molecular dynamics and scattering theory
Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49
A full quantum study of the vibrational predissociation mechanisms in Ar_3^+ cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71
Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $Cs_2NaCeCl_6$, M. Chua and P.A. Tanner 218 (1997) 83

Experimental

Microwave spectroscopy
Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267

Infrared spectroscopy
Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study, B. Tremblay, M.E. Alikhani and L. Manceron 218 (1997) 37
The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277
Infrared spectroscopy of aniline–X (X = N_2, CH_4, CHF_3, CO) clusters and their corresponding cluster cations in the NH_2-stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291

Raman spectroscopy
Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $Cs_2NaCeCl_6$, M. Chua and P.A. Tanner 218 (1997) 83

Visible and UV spectroscopy
Simulation of the SiH ($A^2\Delta \rightarrow X\,^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulias 218 (1997) 57
Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127

The electronic structure of 4-(N,N-dimethylamino)-4′-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
Reverse saturable absorption in palladium and zinc tetraphenyltetrabenzoporphyrin doped xerogels, M. Brunel, F. Chaput, S.A. Vinogradov, B. Campagne, M. Canva, J.P. Boilot and A. Brun 218 (1997) 301

Fluorescence spectroscopy
The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmannsröben 218 (1997) 175
Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H_2, E.R. Wouters, L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande 218 (1997) 309

Electron impact spectroscopy
Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109
Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127

Laser methods
Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $Cs_2NaCeCl_6$, M. Chua and P.A. Tanner 218 (1997) 83
Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211
Intermolecular vibrations of the van der Waals complex p-$C_6H_4FCH_3$...Ar, Y. Hu, W. Lu and S. Yang 218 (1997) 325

Synchrotron spectroscopies
Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199

Multiple resonance spectroscopy
Infrared spectroscopy of aniline–X (X = N_2, CH_4, CHF_3, CO) clusters and their corresponding cluster cations in the NH_2-stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291

Atomic and molecular beam techniques
Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
Intermolecular vibrations of the van der Waals complex p-$C_6H_4FCH_3$...Ar, Y. Hu, W. Lu and S. Yang 218 (1997) 325

Time-resolved experiments
The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmannsröben 218 (1997) 175
Hole transport in vapor deposited enamines and enamine doped polymers, J.A. Sinicropi, J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger 218 (1997) 331

Mass spectrometry
Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
Intermolecular vibrations of the van der Waals complex p-$C_6H_4FCH_3$ ... Ar, Y. Hu, W. Lu and S. Yang 218 (1997) 325

Field emission and field ionization
Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211

Objects

Bulk systems

Supersonic beams
A full quantum study of the vibrational predissociation mechanisms in Ar_3^+ cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71

Liquids neat
Thermodynamic shift from three- to two-dimensional systems, F. Cuadros, A. Mulero and W. Okrasinski 218 (1997) 235

Liquid mixtures and solutions
Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49

Crystals

-neat
Nature of the magnetic interaction of Wurster's radicals in the solid state, F. Dietz, N. Tyutyulkov, C. Christen and K. Lüders 218 (1997) 43

Glasses
The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277

Polymers
Hole transport in vapor deposited enamines and enamine doped polymers, J.A. Sinicropi, J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger 218 (1997) 331

Surfaces
Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
Theoretical study on adsorption and proton exchange reaction of H_2O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257

Plasmas
Simulation of the SiH ($A^2\Delta \rightarrow X\,^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulias 218 (1997) 57

Biological systems
Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225

Microscopic systems

Molecules (neutral and ionic)
Vibrational spectrum and structure of LiOSi. An infrared matrix isolation and density functional theory study, B. Tremblay, M.E. Alikhani and L. Manceron 218 (1997) 37
Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
Theoretical study on adsorption and proton exchange reaction of H_2O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257

-diatomic
Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1
Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH^- and NeH^+, J. Vojtík and J. Fišer 218 (1997) 13
Simulation of the SiH ($A^2\Delta \rightarrow X\,^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulias 218 (1997) 57
Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H_2, E.R. Wouters, L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande 218 (1997) 309

-small polyatomics
Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87
Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109

Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127
Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199

-aromatics
The electronic structure of 4-(N,N-dimethylamino)-4′-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmannsröben 218 (1997) 175
Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191
Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211
The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277

-other large
Reverse saturable absorption in palladium and zinc tetraphenyltetrabenzoporphyrin doped xerogels, M. Brunel, F. Chaput, S.A. Vinogradov, B. Campagne, M. Canva, J.P. Boilot and A. Brun 218 (1997) 301

Molecular aggregates

-van der Waals molecules
Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
Infrared spectroscopy of aniline–X ($X = N_2$, CH_4, CHF_3, CO) clusters and their corresponding cluster cations in the NH_2-stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291
Intermolecular vibrations of the van der Waals complex p-$C_6H_4FCH_3$ ... Ar, Y. Hu, W. Lu and S. Yang 218 (1997) 325

-clusters
Carbon–oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
A full quantum study of the vibrational predissociation mechanisms in Ar_3^+ cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71
Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163
Infrared spectroscopy of aniline–X ($X = N_2$, CH_4, CHF_3, CO) clusters and their corresponding cluster cations in the NH_2-stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291

-complexes
Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
Calculated thermodynamics of reactions involving $NO^+ \cdot X$ complexes (where $X = H_2O$, N_2 and CO_2), P. Mack, J.M. Dyke and T.G. Wright 218 (1997) 243

Defects and impurities
Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225

Ions and charge carriers
Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31

Phenomena

Molecular structure
Carbon–oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
Microsolvation of Cl anion by water clusters: Perturbative Monte Carlo simulations using a hybrid HF/MM potential, T.N. Truong and E.V. Stefanovich 218 (1997) 31
Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267

Vibrations and rotations of molecules
Molecular dynamics simulation of NaCl solutions in methanol–water mixtures. Intramolecular vibrations of the solvent components, E. Hawlicka and D. Swiatla-Wojcik 218 (1997) 49
Construction of a molecular beam Fourier transform microwave spectrometer used to study the 2,5-dihydrofuran–argon van der Waals complex, J.L. Alonso, F.J. Lorenzo, J.C. López, A. Lesarri, S. Mata and H. Dreizler 218 (1997) 267
Intermolecular vibrations of the van der Waals complex p-$C_6H_4FCH_3$ ... Ar, Y. Hu, W. Lu and S. Yang 218 (1997) 325

Electronic structure and states
Carbon–oxygen clusters as hypothetical high energy-density materials, S. Evangelisti 218 (1997) 21
Simulation of the SiH ($A^2\Delta \rightarrow X\,^2\Pi$) emission spectrum in a silane glow discharge and derivation of an improved set of molecular constants, S. Stamou, D. Mataras and D. Rapakoulias 218 (1997) 57
Direct calculation of electronic Raman scattering intensity for Ce^{3+} in $Cs_2NaCeCl_6$, M. Chua and P.A. Tanner 218 (1997) 83
The electronic structure of 4-(N,N-dimethylamino)-4′-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151
Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199

Electric and magnetic properties

Rovibrational dependence of the nuclear quadrupole coupling constants of HF, OH^- and NeH^+, J. Vojtík and J. Fišer 218 (1997) 13

Nature of the magnetic interaction of Wurster's radicals in the solid state, F. Dietz, N. Tyutyulkov, C. Christen and K. Lüders 218 (1997) 43

Spin splittings

Observation of fine structure and hyperfine structure depolarization in the photofragment anisotropy in triplet H_2, E.R. Wouters, L.D.A. Siebbeles, K.L. Reid, B. Buijsse and W.J. van der Zande 218 (1997) 309

Optical activity

The influence of the interaction of carbonyl compounds with the matrix walls on phosphorescence of their solution in porous glasses, S.A. Bagnich 218 (1997) 277

Molecular interactions

Infrared spectroscopy of aniline–X (X = N_2, CH_4, CHF_3, CO) clusters and their corresponding cluster cations in the NH_2-stretching vibration region, R.P. Schmid, P.K. Chowdhury, J. Miyawaki, F. Ito, K. Sugawara, T. Nakanaga, H. Takeo and H. Jones 218 (1997) 291

Spectral bandshapes and intensities

Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87

Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109

Absolute photoabsorption and photoionization studies of methyl bromide using dipole electron impact and synchrotron radiation PES technique, T.N. Olney, G. Cooper, W.F. Chan, G.R. Burton, C.E. Brion and K.H. Tan 218 (1997) 127

Symmetry adapted basis defect patterns for analysis of the effects of energy disorder on cyclic arrays of coupled chromophores, H.-M. Wu and G.J. Small 218 (1997) 225

Energy transfer processes

Lie algebraic method for vibrational and rotational transitions in inelastic collisions of a molecule with a solid surface, D. Guan, X. Yi, S. Ding and B. Yang 218 (1997) 1

Molecular photophysical processes

Quantitative studies of the photoabsorption and photoionization of PCl_3 in the valence and inner (P 2p,2s; Cl 2p,2s) shell regions, J.W. Au and C.E. Brion 218 (1997) 87

Absolute oscillator strengths for the valence-shell photoabsorption (2–200 eV) and the molecular and dissociative photoionization (11–80 eV) of nitrogen dioxide, J.W. Au and C.E. Brion 218 (1997) 109

Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191

Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211

Intramolecular dynamics

-vibrational energy redistribution (including vibrational dissociation)

A full quantum study of the vibrational predissociation mechanisms in Ar_3^+ cluster, E. Buonomo, F.A. Gianturco, M. Pilar de Lara, S. Miret-Artés, G. Delgado-Barrio and P. Villarreal 218 (1997) 71

Reactions (including dissociation)

Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163

Calculated thermodynamics of reactions involving $NO^+ \cdot X$ complexes (where $X = H_2O$, N_2 and CO_2), P. Mack, J.M. Dyke and T.G. Wright 218 (1997) 243

Theoretical study on adsorption and proton exchange reaction of H_2O on H-form zeolite, N. Tajima, T. Taketsugu and K. Hirao 218 (1997) 257

-gas phase

Photodissociation spectroscopy of ICN in the vacuum ultraviolet region, K. Kanda, S. Katsumata, T. Nagata, T. Kondow, A. Hiraya, K. Tabayashi and K. Shobatake 218 (1997) 199

Electron transfer

The electronic structure of 4-(N,N-dimethylamino)-4′-cyano-biphenyl and its planar and twisted model compounds, M. Maus and W. Rettig 218 (1997) 151

The deactivation of singlet excited *all-trans*-1,6-diphenylhexa-1,3,5-triene by charge transfer processes. 2. Formation and dynamics of charge transfer (CT) intermediates, F. Schael, J. Küster and H.-G. Löhmannsröben 218 (1997) 175

Hole transport in vapor deposited enamines and enamine doped polymers, J.A. Sinicropi, J.R. Cowdery-Corvan, E.H. Magin and P.M. Borsenberger 218 (1997) 331

Ionization (including Rydberg states)

Temperature of neutral clusters produced in a seeded molecular beam, and energy transfer during the photoionization process, Ph. Dugourd, D. Rayane, R. Antoine and M. Broyer 218 (1997) 163

Photoionization/dissociation of alkyl substituted benzene molecules using intense near-infrared radiation, M.J. DeWitt, D.W. Peters and R.J. Levis 218 (1997) 211

Fluctuations and noise

Application of the antibunching in dye fluorescence: measuring the excitation rates in solution, Ü. Mets, J. Widengren and R. Rigler 218 (1997) 191